

# 2-Butyn-1-yl chloroformate

<b>Inchi:</b>	InChI=1S/C5H5ClO2/c1-2-3-4-8-5(6)7/h4H2,1H3
<b>InchiKey:</b>	MFKKPMUEGDJJSJL-UHFFFAOYSA-N
<b>Formula:</b>	C5H5ClO2
<b>SMILES:</b>	CC#CCOC(=O)Cl
<b>Mol. weight [g/mol]:</b>	132.54
<b>CAS:</b>	202591-85-3

## Physical Properties

Property code	Value	Unit	Source
gf	-51.83	kJ/mol	Joback Method
hf	-134.77	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.385		Crippen Method
mvol	92.390	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
tb	436.52	K	Joback Method
tc	649.34	K	Joback Method
tf	354.29	K	Joback Method
vc	0.350	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.23	J/molxK	436.52	Joback Method
cpg	163.79	J/molxK	471.99	Joback Method
cpg	170.14	J/molxK	507.46	Joback Method
cpg	176.27	J/molxK	542.93	Joback Method
cpg	182.16	J/molxK	578.40	Joback Method
cpg	187.82	J/molxK	613.87	Joback Method
cpg	193.23	J/molxK	649.34	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C202591853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C202591853&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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